

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.14e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.80e-01

Confidence level: 4.43e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Aniline</div> <div>Measured: 1.58e-02</div> <div>Predicted: 2.83e-01</div>	<div>Image not found</div> <div>Diethyl ethylphosphonate</div> <div>Measured: 3.93e-01</div> <div>Predicted: 1.12e-01</div>	<div>Image not found</div> <div>Linalyl acetate</div> <div>Measured: 6.13e-02</div> <div>Predicted: 8.66e-02</div>
<div>Image not found</div> <div>Amphetamine</div> <div>Measured: 2.00e-04</div> <div>Predicted: 1.09e-01</div>	<div>Image not found</div> <div>Chlorobenzilate</div> <div>Measured: 8.50e-01</div> <div>Predicted: 5.56e-07</div>	